

Wiener index of iterated line graphs of trees homeomorphic to the claw $K_{1,3}$

Martin Knor

Department of Mathematics, Faculty of Civil Engineering, Slovak University of Technology, Radlinského 11, 813 68, Bratislava, Slovakia

Primož Potočnik, Riste Škrekovski

Faculty of Mathematics and Physics, University of Ljubljana, and Institute of Mathematics, Physics and Mechanics, Jadranska 21, 1111 Ljubljana, Slovenia

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Abstract

Let G be a graph. Denote by $L^i(G)$ its i -iterated line graph and denote by $W(G)$ its Wiener index. Dobrynin, Entringer and Gutman stated the following problem: Does there exist a non-trivial tree T and $i \geq 3$ such that $W(L^i(T)) = W(T)$? In a series of five papers we solve this problem. In a previous paper we proved that $W(L^i(T)) > W(T)$ for every tree T that is not homeomorphic to a path, claw $K_{1,3}$ and to the graph of “letter H ”, where $i \geq 3$. Here we prove that $W(L^i(T)) > W(T)$ for every tree T homeomorphic to the claw, $T \neq K_{1,3}$ and $i \geq 4$.

Keywords: Wiener index, iterated line graph, tree, claw.

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1 Introduction

Let G be a graph. For any two of its vertices, say u and v , denote by $d_G(u, v)$ (or by $d(u, v)$ if no confusion is likely) the distance from u to v in G . The Wiener index of G , $W(G)$, is defined as

$$W(G) = \sum_{u \neq v} d(u, v),$$

where the sum is taken through all unordered pairs of vertices of G . Wiener index was introduced by Wiener in [12]. It is related to boiling point, heat of evaporation, heat of

E-mail addresses: knor@math.sk (Martin Knor) primoz.potocnik@fmf.uni-lj.si (Primož Potočnik), skrekovski@gmail.com (Riste Škrekovski),

formation, chromatographic retention times, surface tension, vapour pressure, partition coefficients, total electron energy of polymers, ultrasonic sound velocity, internal energy, etc., see [8]. For this reason Wiener index is widely studied by chemists. The interest of mathematicians was attracted in 1970's. It was reintroduced as the distance and transmission, see [5] and [11], respectively. Recently, there are whole special issues of journals devoted to (mathematical properties) of Wiener index, see [6] and [7], as well as several surveys, see e.g. [3] and [4].

By definition, if G has a unique vertex, then $W(G) = 0$. In this case, we say that the graph G is *trivial*. We set $W(G) = 0$ also when the set of vertices (and hence also the set of edges) of G is empty.

The line graph of G , $L(G)$, has vertex set identical with the set of edges of G . Two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G . Iterated line graphs are defined inductively as follows:

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

In [1] we have the following statement.

Theorem 1.1. Let T be a tree on n vertices. Then $W(L(T)) = W(T) - \binom{n}{2}$.

Since $\binom{n}{2} > 0$ if $n \geq 2$, there is no nontrivial tree for which $W(L(T)) = W(T)$. However, there are trees T satisfying $W(L^2(T)) = W(T)$, see e.g. [2]. In [3], the following problem was posed:

Problem 1.2. Is there any tree T satisfying the equality $W(L^i(T)) = W(T)$ for some $i \geq 3$?

As observed above, if T is a trivial tree then $W(L^i(T)) = W(T)$ for every $i \geq 1$, although here the graph $L^i(T)$ is empty.

Denote by H the tree on six vertices out of which two have degree 3 and four have degree 1. Since H can be drawn to resemble the letter H , it is often called the H -graph. Graphs G_1 and G_2 are homeomorphic if and only if the graphs obtained from G_1 and G_2 , respectively, by substituting the vertices of degree two together with the two incident edges with a single edge, are isomorphic. In [10] we proved the following:

Theorem 1.3. Let T be a tree, not homeomorphic to a path, claw $K_{1,3}$ and the graph H . Then $W(L^i(T)) > W(T)$ for all $i \geq 3$.

Since the case when T is a path is trivial, it remains to consider graphs homeomorphic to the claw $K_{1,3}$ and those homeomorphic to H . In this paper we concentrate on graphs homeomorphic to the claw $K_{1,3}$. The remaining two cases, namely the trees homeomorphic to H for $i \geq 3$ and trees homeomorphic to $K_{1,3}$ for $i = 3$, are dealt with in a forthcoming paper.

First, consider the case of the claw $K_{1,3}$ itself. Then $L^i(K_{1,3})$ is a cycle of length 3 for every $i \geq 1$. Since $W(K_{1,3}) = 9$ and the Wiener index of the cycle of length 3 is 3, we have $W(L^i(K_{1,3})) < W(K_{1,3})$ for every $i \geq 1$. For other trees homeomorphic to $K_{1,3}$, we prove the opposite inequality, provided that $i \geq 4$:

Theorem 1.4. Let T be a tree homeomorphic to $K_{1,3}$, such that $T \neq K_{1,3}$. Then it holds that $W(L^i(T)) > W(T)$ for every $i \geq 4$.

In [9] we proved the following statement:

Theorem 1.5. Let G be a connected graph. Then $f_G(i) = W(L^i(G))$ is a convex function in variable i .

Hence, to prove Theorem 1.4 it suffices to prove:

Theorem 1.6. Let T be a tree homeomorphic to $K_{1,3}$, such that $T \neq K_{1,3}$. Then it holds $W(L^4(T)) > W(T)$.

2 Proofs

Let $a, b, c \geq 1$. Denote by $C_{a,b,c}$ a tree that has three paths of lengths a, b and c , starting at a common vertex of degree 3. Obviously, $C_{a,b,c}$ is homeomorphic to $K_{1,3}$ and $C_{1,1,1} = K_{1,3}$. By symmetry, we may assume $a \geq b \geq c$, see Figure 1 for $C_{5,4,3}$.

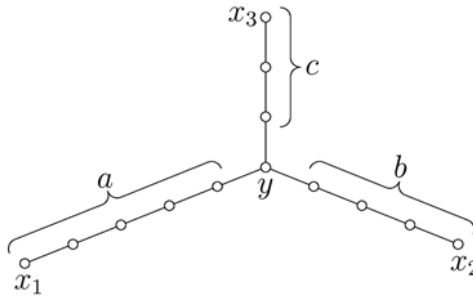


Figure 1: The graph $C_{5,4,3}$.

Denote

$$\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}).$$

Our aim is to prove $\Delta C_{a,b,c} > 0$ if $a \geq 2$. We start with the case $a \leq 3$. This case will serve as the base of induction in the proof of Theorem 1.6.

Lemma 2.1. Let $3 \geq a \geq b \geq c \geq 1$ and $a \neq 1$. Then $\Delta C_{a,b,c} > 0$.

Proof. Since $3 \geq a \geq b \geq c \geq 1$ and $a \neq 1$, there are 9 cases to consider. In Table 1 we present $\Delta C_{a,b,c}$ for each of these cases. The results were found by a computer, though it is rather easy to find $W(C_{a,b,c})$ by hand, and $W(L^4(C_{a,b,c}))$ can be found by applying Proposition 2.3 to $L^2(C_{a,b,c})$. □

(a, b, c)	$W(C_{a,b,c})$	$W(L^4(C_{a,b,c}))$	$\Delta C_{a,b,c}$
(3, 3, 3)	138	642	504
(3, 3, 2)	102	533	431
(3, 3, 1)	75	257	182
(3, 2, 2)	72	435	363
(3, 2, 1)	50	192	142
(3, 1, 1)	32	65	33
(2, 2, 2)	48	348	300
(2, 2, 1)	31	138	107
(2, 1, 1)	18	38	20

Table 1: $\Delta C_{a,b,c}$ for $a \leq 3$.

In what follows we assume that $a \geq 4$. Denote

$$\begin{aligned} \delta_0(a, b, c) &= W(C_{a,b,c}) - W(C_{a-1,b,c}) \\ \delta_4(a, b, c) &= W(L^4(C_{a,b,c})) - W(L^4(C_{a-1,b,c})). \end{aligned}$$

Then

$$\Delta C_{a,b,c} - \Delta C_{a-1,b,c} = \delta_4(a, b, c) - \delta_0(a, b, c), \tag{2.1}$$

so if we prove $\delta_4(a, b, c) - \delta_0(a, b, c) \geq 0$, we obtain $\Delta C_{a,b,c} \geq \Delta C_{a-1,b,c}$.

We distinguish 4 vertices in $C_{a,b,c}$. Denote by y the vertex of degree 3, and denote by x_1, x_2 and x_3 the pendant vertices so that $d(x_1, y) = a, d(x_2, y) = b$ and $d(x_3, y) = c$, see Figure 1. As is the custom, by $V(G)$ we denote the vertex set of G .

Lemma 2.2. Let $a, b, c \geq 1$. Then

$$\delta_0(a, b, c) = \binom{a+b+1}{2} + \binom{a+c+1}{2} - \binom{a+1}{2}.$$

Proof. Since $C_{a-1,b,c}$ is a subgraph of $C_{a,b,c}$ with $V(C_{a,b,c}) - V(C_{a-1,b,c}) = \{x_1\}$, we have

$$\delta_0(a, b, c) = W(C_{a,b,c}) - W(C_{a-1,b,c}) = \sum_u d(u, x_1),$$

where the sum goes through all $u \in V(C_{a,b,c}) \setminus \{x_1\}$. For vertices u of the $x_1 - x_2$ path, the sum of all $d(u, x_1)$ is $1 + 2 + \dots + (a+b) = \binom{a+b+1}{2}$. For vertices of the $x_1 - x_3$ path which do not lay on $x_1 - x_2$ path, the sum of $d(u, x_1)$ is $(a+1) + (a+2) + \dots + (a+c) = \binom{a+c+1}{2} - \binom{a+1}{2}$, see Figure 1. Since the paths $x_1 - x_2$ and $x_1 - x_3$ contain all vertices of $C_{a,b,c}$, we have $\delta_0(a, b, c) = \binom{a+b+1}{2} + \binom{a+c+1}{2} - \binom{a+1}{2}$. \square

For two subgraphs S_1 and S_2 of G , by $d(S_1, S_2)$ we denote the shortest distance in G between a vertex of S_1 and a vertex of S_2 . If S_1 and S_2 share an edge then we set $d(S_1, S_2) = -1$.

Analogously as a vertex of $L(G)$ corresponds to an edge of G , a vertex of $L^2(G)$ corresponds to a path of length two in G . For $x \in V(L^2(G))$ we denote by $B_2(x)$ the corresponding path in G . Let x and y be two distinct vertices of $L^2(G)$. It was proved in [9] that

$$d_{L^2(G)}(x, y) = d_G(B_2(x), B_2(y)) + 2.$$

Let $u, v \in V(G)$, $u \neq v$. Denote by $\beta_i(u, v)$ the number of pairs $x, y \in V(L^2(G))$, with u being the center of $B_2(x)$ and v being the center of $B_2(y)$, such that $d(B_2(x), B_2(y)) = d(u, v) - 2 + i$. Since $d(u, v) - 2 \leq d(B_2(x), B_2(y)) \leq d(u, v)$, we have $\beta_i(u, v) = 0$ for all $i \notin \{0, 1, 2\}$. Denote by $\deg(w)$ the degree of w in G . In [9] we have the following statement:

Proposition 2.3. *Let G be a connected graph. Then*

$$\begin{aligned}
 W(L^2(G)) &= \sum_{u \neq v} \left[\binom{\deg(u)}{2} \binom{\deg(v)}{2} d(u, v) + \beta_1(u, v) + 2\beta_2(u, v) \right] \\
 &+ \sum_u \left[3 \binom{\deg(u)}{3} + 6 \binom{\deg(u)}{4} \right], \tag{2.2}
 \end{aligned}$$

where the first sum goes through unordered pairs $u, v \in V(G)$ and the second one goes through $u \in V(G)$.

We apply Proposition 2.3 to $L^2(C_{a,b,c})$ and $L^2(C_{a-1,b,c})$. This enables us to calculate $\delta_4(a, b, c)$ using degrees and distances of the second iterated line graph.

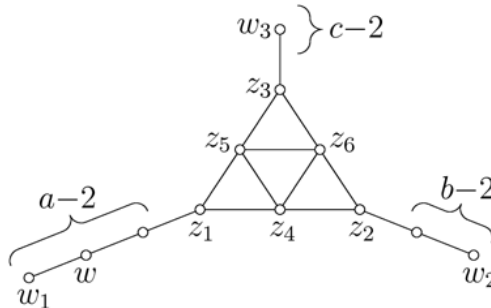


Figure 2: The graph $L^2(C_{5,4,3})$.

Denote by w_1 the pendant vertex of $L^2(C_{a,b,c})$ corresponding to the path of length 2 terminating at x_1 . Since $a \geq 4$, the unique neighbour of w_1 has degree 2. Denote by w this neighbour, see Figure 2. For every vertex $u \in V(L^2(C_{a,b,c})) \setminus \{w, w_1\}$, denote by $n(u)$ the number of neighbours of u , whose distance to w is at least $d(u, w)$. We have:

Lemma 2.4. Let $a \geq 4$ and $b, c \geq 1$. Then

$$\delta_4(a, b, c) = \sum_u \left[\binom{\deg(u)}{2} d(u, w) + \binom{n(u)}{2} \right],$$

where the sum goes through all vertices of $V(L^2(C_{a,b,c})) \setminus \{w, w_1\}$.

PROOF. Observe that $L^2(C_{a-1,b,c})$ is a subgraph of $L^2(C_{a,b,c})$ and $V(L^2(C_{a,b,c})) \setminus V(L^2(C_{a-1,b,c})) = \{w_1\}$. Since $\deg(w_1) = 1$, the vertex w_1 cannot be the center of a path of length 2, implying that $\beta_i(u, w_1) = 0$ for every u and i . Since $\binom{\deg(w_1)}{2} =$

0, all summands of (2.2) containing w_1 contribute 0 to $W(L^4(C_{a,b,c}))$. The vertices of $L^2(C_{a-1,b,c})$, except w , have the same degree in $L^2(C_{a,b,c})$ as in $L^2(C_{a-1,b,c})$. The degree of w is 1 in $L^2(C_{a-1,b,c})$, and it is 2 in $L^2(C_{a,b,c})$. Therefore $\sum_u [3 \binom{\deg(u)}{3} + 6 \binom{\deg(u)}{4}]$ has the same value in $L^2(C_{a,b,c})$ as in $L^2(C_{a-1,b,c})$, so these sums will cancel out. Thus, we have

$$\begin{aligned} \delta_4(a, b, c) &= W(L^2(L^2(C_{a,b,c}))) - W(L^2(L^2(C_{a-1,b,c}))) \\ &= \sum_u \left[\binom{\deg(u)}{2} \binom{2}{2} d(u, w) + \beta_1(u, w) + 2\beta_2(u, w) \right], \end{aligned}$$

where the sum goes through $u \in V(L^2(C_{a-1,b,c})) \setminus \{w\}$.

Let $u \in V(L^2(C_{a-1,b,c})) \setminus \{w\}$. Since $\deg(w_1) = 1$ and $\deg(w) = 2$ in $L^2(C_{a,b,c})$, the unique path of length 2 centered at w contains an endvertex closer to u than w . Hence, $\beta_2(u, w) = 0$. Consequently, $\beta_1(u, w)$ equals the number of paths of length 2 centered at u , both endvertices of which have distance to w at least $d(u, w)$. Hence, $\beta_1(u, w) = \binom{n(u)}{2}$, which completes the proof. \square

Using Lemma 2.4 we prove the induction step.

Lemma 2.5. Let $a \geq b \geq c \geq 1$ and $a \geq 4$. Then $\delta_4(a, b, c) \geq \delta_0(a, b, c)$.

Proof. We distinguish 8 more vertices in $L^2(C_{a,b,c})$. Denote by w_2 and w_3 pendant vertices corresponding to the paths of length 2 containing x_2 and x_3 , respectively, see Figure 1 and 2. Denote by z_1, z_2 and z_3 the vertices corresponding to the paths of length 2, whose endvertex is y ; and denote by z_4, z_5 and z_6 the vertices corresponding to the paths of length 2 centered at y . Of course, if $b \leq 2$ or $c \leq 2$, then some of these vertices are not defined.

For $u \in V(L^2(C_{a-1,b,c})) \setminus \{w\}$, denote

$$h(u) = \binom{\deg(u)}{2} d(u, w) + \binom{n(u)}{2}.$$

By Lemma 2.4, we have $\delta_4(a, b, c) = \sum_u h(u)$, where the sum goes through all vertices of $V(L^2(C_{a,b,c})) \setminus \{w, w_1\}$. If $u \in \{w_2, w_3\}$ then $\deg(u) = 1$ and $n(u) = 0$, so $h(u) = 0$. Thus, vertices of degree 1 contribute 0 to $\sum_u h(u)$. Denote

$$S_i = \sum_u h(u),$$

where the sum is taken over all interior vertices u of the $w_i - z_i$ path, $u \neq w$ and $1 \leq i \leq 3$. Then $\delta_4(a, b, c) = \sum_{i=1}^3 S_i + \sum_{i=1}^6 h(z_i)$.

Regarding the values of a, b and c , we distinguish 4 cases:

Case 1. $a \geq 4$ and $b, c \geq 3$.

If u is a vertex of degree 2, then $n(u) = 1$ and $\binom{\deg(u)}{2} = 1$. Hence $h(u) = d(u, w)$. Thus,

$$\begin{aligned} S_1 &= 1 + 2 + \dots + (a-4) = \binom{a-3}{2} \\ S_2 &= a + (a+1) + \dots + (a+b-4) = \binom{a+b-3}{2} - \binom{a}{2} \\ S_3 &= a + (a+1) + \dots + (a+c-4) = \binom{a+c-3}{2} - \binom{a}{2}. \end{aligned}$$

If $u \in \{z_1, z_2, z_3\}$, then $\deg(u) = 3$ and $n(u) = 2$. Thus $h(u) = 3d(u, w) + 1$. If $u \in \{z_4, z_5\}$, then $\deg(u) = 4$ and $n(u) = 3$, so $h(u) = 6d(u, w) + 3$. Finally, if $u = z_6$, then $\deg(u) = 4$ and $n(u) = 2$, so $h(u) = 6d(u, w) + 1$. This gives

$$\begin{aligned} h(z_1) &= 3(a-3) + 1 & h(z_4) &= h(z_5) = 6(a-2) + 3 \\ h(z_2) &= h(z_3) = 3(a-1) + 1 & h(z_6) &= 6(a-1) + 1. \end{aligned}$$

Since $\delta_4(a, b, c) = \sum_{i=1}^3 S_i + \sum_{i=1}^6 h(z_i)$, we have

$$\begin{aligned} \delta_4(a, b, c) &= \binom{a-3}{2} + \binom{a+b-3}{2} + \binom{a+c-3}{2} - 2\binom{a}{2} \\ &\quad + (3a-8) + 2(3a-2) + 2(6a-9) + (6a-5). \end{aligned}$$

Denote $P = \delta_4(a, b, c) - \delta_0(a, b, c)$. By Lemma 2.2 we have $\delta_0(a, b, c) = \binom{a+b+1}{2} + \binom{a+c+1}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 17a - 4b - 4c - 17.$$

Since $a \geq b$ and $a \geq c$, we have $P \geq 9a - 17$. Finally, since $a \geq 4$, we have $P = \delta_4(a, b, c) - \delta_0(a, b, c) \geq 0$.

Case 2. $a \geq 4, b \geq 3$ and $c \leq 2$.

We calculate first $\delta_4(a, b, 1)$. In $L^2(C_{a,b,1})$ we have $S_3 = 0$; note that z_3 is not defined here and that $\deg(z_5) = \deg(z_6) = 3$ (see Figure 2). Analogously as in Case 1 we get:

$$\begin{aligned} S_1 &= \binom{a-3}{2} & h(z_2) &= 3(a-1) + 1 \\ S_2 &= \binom{a+b-3}{2} - \binom{a}{2} & h(z_4) &= 6(a-2) + 3 \\ S_3 &= 0 & h(z_5) &= 3(a-2) + 1 \\ h(z_1) &= 3(a-3) + 1 & h(z_6) &= 3(a-1) \end{aligned}$$

since $n(z_5) = 2$ and $n(z_6) = 1$. Thus,

$$\begin{aligned} \delta_4(a, b, 1) &= \binom{a-3}{2} + \binom{a+b-3}{2} - \binom{a}{2} + (3a-8) \\ &\quad + (3a-2) + (6a-9) + (3a-5) + (3a-3). \end{aligned}$$

Denote $P = \delta_4(a, b, 1) - \delta_0(a, b, 2)$. By Lemma 2.2 we have $\delta_0(a, b, 2) = \binom{a+b+1}{2} + \binom{a+3}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 9a - 4b - 18.$$

Since $a \geq b$, we have $P \geq 5a - 18$, and as $a \geq 4$, we have $P \geq 0$. Since $\delta_4(a, b, 2) \geq \delta_4(a, b, 1)$ and $\delta_0(a, b, 2) \geq \delta_0(a, b, 1)$, we conclude $\delta_4(a, b, i) - \delta_0(a, b, i) \geq P \geq 0$ for $i \in \{1, 2\}$.

Case 3. $a \geq 4, b = 2$ and $c \leq 2$.

We find $\delta_4(a, 2, 1)$. In $L^2(C_{a,2,1})$ we have $S_2 = S_3 = 0$. Again, the vertex z_3 is not defined here, $\deg(z_2) = 2$ and $\deg(z_5) = \deg(z_6) = 3$ (see Figure 2). Analogously as in the previous cases we get:

$$\begin{aligned} S_1 &= \binom{a-3}{2} & h(z_4) &= 6(a-2) + 3 \\ h(z_1) &= 3(a-3) + 1 & h(z_5) &= 3(a-2) + 1 \\ h(z_2) &= (a-1) & h(z_6) &= 3(a-1) \end{aligned}$$

since $n(z_2) = 1$, $n(z_5) = 2$ and $n(z_6) = 1$. Thus,

$$\delta_4(a, 2, 1) = \binom{a-3}{2} + (3a-8) + (a-1) + (6a-9) + (3a-5) + (3a-3).$$

Denote $P = \delta_4(a, 2, 1) - \delta_0(a, 2, 2)$. By Lemma 2.2 we have $\delta_0(a, 2, 2) = 2\binom{a+3}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 8a - 26.$$

Since $a \geq 4$, we have $P \geq 0$. Since $\delta_4(a, 2, 2) \geq \delta_4(a, 2, 1)$ and $\delta_0(a, 2, 2) \geq \delta_0(a, 2, 1)$, we conclude $\delta_4(a, 2, i) - \delta_0(a, 2, i) \geq P \geq 0$ for $i \in \{1, 2\}$.

Case 4. $a \geq 4$ and $b = c = 1$.

In $L^2(C_{a,1,1})$ we have $S_2 = S_3 = 0$. Note that the vertices z_2 and z_3 are not defined, while $\deg(z_4) = \deg(z_5) = 3$ and $\deg(z_6) = 2$ (see Figure 2). Analogously as in the previous cases we get:

$$\begin{aligned} S_1 &= \binom{a-3}{2} & h(z_4) &= h(z_5) = 3(a-2) + 1 \\ h(z_1) &= 3(a-3) + 1 & h(z_6) &= (a-1) \end{aligned}$$

since $n(z_4) = n(z_5) = 2$ and $n(z_6) = 0$. Thus,

$$\delta_4(a, 1, 1) = \binom{a-3}{2} + (3a-8) + 2(3a-5) + (a-1).$$

Denote $P = \delta_4(a, 1, 1) - \delta_0(a, 1, 1)$. By Lemma 2.2 we have $\delta_0(a, 1, 1) = 2\binom{a+2}{2} - \binom{a+1}{2}$. Expanding the terms we get

$$P = 4a - 15.$$

Since $a \geq 4$, we have $P \geq 0$, and hence $\delta_4(a, 1, 1) - \delta_0(a, 1, 1) \geq P \geq 0$. □

Proof of Theorem 1.6. Let T be the tree $C_{a,b,c}$ with $a \geq b \geq c \geq 1$, such that $a \neq 1$. If $a \leq 3$, then $\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}) > 0$, by Lemma 2.1.

Now suppose that $a \geq 4$. Consider lexicographical ordering of triples (a', b', c') with $a' \geq b' \geq c' \geq 1$ and $a' \geq 2$. Further, assume that $\Delta C_{a',b',c'} > 0$ for every triple (a', b', c') , such that $a' \geq b' \geq c' \geq 1$ and $a' \geq 2$, which is in the lexicographical ordering smaller than (a, b, c) .

Let (a^*, b^*, c^*) be ordering of triple $(a-1, b, c)$, such that the multisets $\{a^*, b^*, c^*\}$ and $\{a-1, b, c\}$ are the same and $a^* \geq b^* \geq c^*$. Then $C_{a-1,b,c}$ and C_{a^*,b^*,c^*} are isomorphic graphs. Moreover, since $a \geq 4$, we have $a^* \geq 3$. By (2.1) and Lemma 2.5 we see that

$$\begin{aligned} \Delta C_{a,b,c} - \Delta C_{a^*,b^*,c^*} &= \Delta C_{a,b,c} - \Delta C_{a-1,b,c} \\ &= \delta_4(a, b, c) - \delta_0(a, b, c) \\ &\geq 0. \end{aligned}$$

Since (a^*, b^*, c^*) is in the lexicographical ordering smaller than (a, b, c) and $a^* \geq 2$, by the induction hypothesis we have $\Delta C_{a^*,b^*,c^*} > 0$. Hence, $\Delta C_{a,b,c} = W(L^4(C_{a,b,c})) - W(C_{a,b,c}) > 0$. □

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